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Reactivity of NO and $(NO)_2$ on Cu(110)

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The adsorption of NO on transition metal surfaces in general shows a remarkable variety of possible bonding configurations which raises considerable interest from both chemical and catalytic point of view. The RHF and DFT methods are employed in order to calculate the energy that is required to dissociate the NO molecule from the Cu surface. According to experiment when Cu(110) is exposed to NO in the temperature range 40-85K initial adsorption leads to the presence of molecular NO on the surface. With further exposure to NO this is replaced by the dimeric $(NO)_2$ species. The objective of this work is to calculate the dissociation energy of Cu_xNO and $Cu_x(NO)_2$